CLAIMS

What is claimed is:

1. A method for quantitation of surface-binding optical resonance profiles comprising, in combination, the steps of:

obtaining at least one calibration result from a calibration scan of at least one Region of Interest;

generating, from at least one calibration result, a calibration profile for at least one scanned Region of Interest;

obtaining at least one experimental result from an experimental scan of at least one Region of Interest; and

determining at least one resonance parameter for at least one experimental result relative to at least one calibration profile.

2. The method of claim 1, wherein one resonance parameter is an angle shift.

3. The method of claim 1, wherein one resonance parameter is a wavelength shift.

4. The method of claim 1, further including the step of storing at least one calibration profile in memory.

5. The method of claim 1, further including the step of storing at least one resonance parameter in memory.

6. The method of claim 1, further comprising the step of computing at least one calibration set statistic.

7. The method of claim 6, further including the step of displaying at least one calibration set statistic.

8. The method of claim 1, wherein said step of generating a calibration profile for at least one scanned Region of Interest comprises the steps of:

generating a raw calibration profile; and

determining at least one derivative of said calibration profile from the raw calibration profile.

9. The method of claim 8, wherein said step of generating a calibration profile for at least one scanned Region of Interest further comprises the step of smoothing said raw calibration profile.

10. The method of claim 8, wherein said step of generating a calibration profile for at least one scanned Region of Interest further comprises the step of determining at least one property of said calibration profile from the raw calibration profile.

11. The method of claim 10, wherein the properties determined are selected from the group consisting of Full Width at Half Maximum, nominal resonance angle, fractional depth, and maximum intensity.

12. The method of claim 9, wherein said step of generating a calibration profile further comprises the step of subsampling the smoothed raw calibration profile.

13. The method of claim 12, wherein said step of generating a calibration profile further comprises the step of extrapolating the ends of the subsampled smoothed raw calibration profile.

14. The method of claim 13, wherein said step of generating a calibration profile further comprises the step of performing a second smooth of the subsampled smoothed raw calibration profile.

15. The method of claim 14, wherein said step of generating a calibration profile further comprises the step of storing the calibration profile in memory.

16. The method of claim 15, wherein said step of generating a calibration profile further comprises the steps of:

determining the quality of the calibration profile; and

marking the calibration profile according to the quality determination.

17. The method of claim 1, further including the step of performing a preliminary quality check on at least one calibration result.

18. The method of claim 17, further including the step of flagging at least one calibration result in memory as valid or invalid according to the results of the preliminary quality check.

19. The method of claim 1, further including the step of computing a derivative of at least one calibration profile.

20. The method of claim 1, further including the step of displaying at least one scan result to a user.

21. The method of claim 1, wherein said step of determining at least one resonance parameter for said experimental scan of at least one Region of Interest comprises the steps of:

calculating an estimated resonance shift;

calculating at least one interpolated profile from said estimated resonance shift and said calibration profile;

fitting said experimental scan, using said interpolated calibration profile;

obtaining fit coefficients from said step of fitting;

calculating, from the fit coefficients, a residual resonance shift from the resonance shift;

calculating an improved estimate of the resonance shift; and

iterating until the value of the resonance shift converges to a predetermined convergence criterion.

22. The method of claim 21, wherein said step of determining at least one resonance parameter for said experimental scan of at least one Region of Interest comprises the step of calculating fit residuals.

23. The method of claim 21, wherein said step of determining at least one resonance parameter further includes the step of estimating the time of scan minimum.

24. The method of claim 23, wherein said step of determining at least one resonance parameter further includes the step of initially pruning the experimental scan to within the limits of the calibration profile.

25. The method of claim 24, wherein said step of determining at least one resonance parameter further includes the step of fitting to a sweet zone, comprising the steps of:

truncating the interpolated profile to the sweet zone; and

redetermining the resonance parameter utilizing the truncated interpolated profile.

26. The method of claim 25, wherein said step of determining at least one resonance parameter further includes the step of performing initial data validity checks.

27. The method of claim 26, wherein said step of performing initial data validity checks comprises the steps of:

checking profile availability;

checking self-consistency of data; and

checking scan indexing.

28. The method of claim 21, wherein said step of fitting employs a least squares fit.

29. The method of claim 1, further including the step of reporting errors in an error log.

30. The method of claim 29, wherein the step of reporting errors utilizes a local error log.

31. The method of claim 29, wherein the step of reporting errors employs remote error reporting.

32. The method of claim 1, further including the step of performing a chip qualification check.

33. A method for quantitation of surface-binding optical resonance profiles comprising, in combination, the steps of:

obtaining at least one calibration result from a calibration scan of at least one Region of Interest;

generating, from at least one calibration result, a calibration profile for at least one scanned Region of Interest, comprising the steps of:

generating a raw calibration profile;

smoothing said raw calibration profile;

subsampling the smoothed raw calibration profile; and

determining properties of said calibration profile from the smoothed raw calibration profile;

storing at least one calibration profile in memory;

computing a derivative of at least one calibration profile;

obtaining at least one experimental result from an experimental scan of at least one Region of Interest;

determining a resonance shift of at least one experimental result relative to at least one calibration profile, comprising the steps of:

calculating an estimated resonance shift;

calculating at least one interpolated profile from said estimated resonance shift and said calibration profile;

fitting said experimental scan, using said interpolated calibration profile;

obtaining fit coefficients from said step of fitting;

calculating, from the fit coefficients, a residual resonance shift from the

resonance shift;

calculating an improved estimate of the resonance shift;

calculating fit residuals;

iterating until the estimated value of the resonance shift converges to a predetermined convergence criterion; and

estimating the time of scan minimum; and

displaying at least one scan result to a user.

34. An apparatus for quantitation of surface-binding optical resonance profiles comprising, in combination:

calibration module, said calibration module comprising:

calibration scan result fetcher; and

calibration profile creation module; and

fitting module, said fitting module comprising:

experimental scan result fetcher;

calibration profile fetcher; and

resonance shift determination module.

35. The apparatus of claim 34, wherein said calibration profile creation module further includes a curve smoother.

36. The apparatus of claim 34, wherein said calibration profile creation module further includes a subsampler.

37. The apparatus of claim 34, wherein said calibration profile creation module further includes a curve smoother and a subsampler.

38. The apparatus of claim 34, further including a resonance parameter calculator.

39. The apparatus of claim 38, wherein the calculated resonance parameters are selected from the group consisting of estimated absolute resonance point, time of resonance minimum, diagnostic information, and quality information.

40. The apparatus of claim 34, further including an instrument control and data acquisition module.

41. The apparatus of claim 40, further including a test and support module.

42. A method for qualifying a surface plasmon resonance chip comprising, in combination, the steps of:

obtaining a golden calibration profile for the type of chip to be qualified;

obtaining at least one calibration result from a calibration scan of at least one Region of Interest of a chip to be tested;

comparing said at least one calibration result to said golden calibration profile to obtain at least one comparison result; and

determining whether said chip is suitable for use by applying selection criteria to said at least one comparison result.

43. The method of claim 42, further including the step of displaying chip qualification results to the user.

44. The method of claim 43, wherein the step of determining whether the chip is suitable includes the step of incrementing a "bad ROI" count.

45. The method of claim 44, wherein the step of determining whether the chip is suitable includes the step of storing a "bad ROI" number for display.

46. The method of claim 42, wherein the step of comparing the calibration includes the step of initializing a fit module with a chip qualification parameter set.